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Limit on remote FTIR detection of trace gases

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Abstract

We studied the capability of a Fourier spectrometer system to remotely detect trace gases in localized clouds, e.g., stationary source effluents. Detection is based on the degree to which the observed IR spectral radiance contrast between the cloud and adjacent background is correlated with a computed reference spectrum. It is shown that trace gases can be reliably detected when spectral features are well below the noise level. The minimum detectable quantities (MDQ's) for various trace gases at one atmosphere total pressure are given. The MDQ's determine the combinations of gas column thickness and gas-background temperature difference that correspond to 95 percent detection probability and one percent false detection probability when an FTS system with modest-size foreoptics views the target through a path equivalent to approximately one air mass.

Introduction

Infrared-active trace gases in a localized cloud can be remotely detected on the basis of the contrast they produce in an IR scene image. Of course, the gas temperature and average background brightness temperature must be different, and the resultant spatial radiance contrast must be distinguishable from background clutter. Resolution of the image into many spectral elements will give additional information that can be used to suppress the effects of background clutter, atmospheric spatial variations and system noise, and to distinguish between different trace species in the cloud.

The imaging spectrometer gives the spectrum of the difference between target (trace gas) and background radiances, which can be compared to a computed reference contrast spectrum. Parameters based on the degree of correlation between the two spectra can be used to decide whether a particular target species is present and also to characterize its amount.

From studies reported elsewhere^{1,2} it was decided that a mosaic FTS was the best type of sensor. This choice was based on an assumed target cloud size, detection range and sensitivity requirements (foreoptics size and field of view), the number and spectral locations of the target species IR bands, and the current technology of high-performance detector mosaics. This paper gives, for a particular baseline FTS system, the minimum detectable quantities of 13 molecular species. System noise-equivalent spectral radiances for the detection bands are also given, which allows scaling of the MDQ's with respect to system radiometric parameters. The reported MDQ's correspond to ideal conditions; i.e., it is assumed that system performance is limited by detector (system) noise rather than atmospheric/background variations, and that the reference spectrum (which includes atmospheric spectral absorption effects) is known precisely. The effects of non-ideal conditions are discussed in Ref. 1.

Theoretical basis

It can be shown¹ that the measured spectral radiance contrast, apart from system spectral noise, is

$$\Delta N_v = N_2 - N_1 \approx D \tau_v a_{gv}; \quad D = \frac{u \Delta B_v}{T_g T_{sfc}} \quad (1)$$

where τ_v = atmospheric spectral transmittance between the target and sensor,

a_{gv} = spectral absorption coefficient of the (single) target gas,

u = molecular column thickness of the target gas (number of molecules per unit area in the line-of-sight), and

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$\overline{\Delta B}_v$ = difference between the spectral radiance of a blackbody at the gas temperature T_g and the actual spectral radiance of the background at temperature T_{sfc} , averaged over the detection spectral band.

The detectable quantity, denoted by D , is essentially a scale factor in the measured contrast spectrum. Equation (1) is an approximation only because we have replaced the actual spectral variation ΔB_v by its average value. However, the variation is slow compared to that of τ_v and a_{gv} and is nearly linear over narrow detection bands, so that the approximation is a good one, especially if $\tau_v \approx 1$ and a_{gv} is more-or-less symmetrical about the center of the detection band.

A reasonably accurate theoretical estimate of $\tau_v a_{gv}$ can be obtained using a line-by-line computer code such as AFGL's FASCOD1.³ Then an estimate D' of D can be obtained by finding the value that minimizes the mean square difference between the measured spectrum ΔN_v and $D' \tau_v a_{gv}$. Of course, a_{gv} is a function of the gas temperature, but $\partial \ln a_{gv} / \partial T_g \ll \partial \ln \Delta B_v / \partial T_g$. Hence, the use of some guess temperature in computing a_{gv} will not result in a large error in D' .

Some simple types of background and atmospheric interferences can be suppressed by subtracting the means of ΔN_v and $\tau_v a_{gv}$ from these spectra before they are used to estimate D . The least-squares estimator of D is then

$$D' = \frac{\sum (a - \bar{a})(b - \bar{b})}{\sum (b - \bar{b})^2} \equiv \frac{\sigma_{ab}}{\sigma_b^2} \quad (2)$$

where $a \equiv \Delta N_v + \text{NOISE}_v$, $b \equiv \tau_v a_{gv}$, and the summations are over the digitized spectrum values. Equation (2) is the prescription for computing the estimate D' given the measurement a and reference contrast spectrum b . By combining Eqs. (1) and (2), we find that D' can also be expressed by

$$D' = D + \frac{\sigma_{bn}}{\sigma_b^2}$$

where σ_{bn} is the covariance of the digitized reference spectrum b and the spectrum noise NOISE_v , and σ_b^2 is the variance of the digitized reference spectrum.

The spectrum noise samples will be Gaussian with zero mean, and the samples will also be independent provided the sample spacing is approximately equal to the resolution Δv of the FTS system. It can be shown that if the spacing is Δv the second term of Eq. (3) is

$$\frac{\sigma_{bn}}{\sigma_b^2} = \frac{x \sigma_n}{\sqrt{M} \sigma_b} = x \frac{\sqrt{2} \text{NESR}}{\sqrt{M} \sigma_b} \equiv x \sigma_D \quad (4)$$

where x is a unit normal random variate, M is the total number of resolved spectral elements in the spectra a and b , and NESR is the average system noise-equivalent spectral radiance over the detection band. Note that the effective rms noise σ_n equals $\sqrt{2} \text{NESR}$ because ΔN_v is the difference of two measurements with independent noise. Thus, the rms uncertainty in D' is $\sigma_D \equiv \sqrt{2} \text{NESR} / (\sqrt{M} \sigma_b)$.

The quantity

$$\frac{\sigma_{bD}}{\sqrt{2} \text{NESR}} \equiv \frac{S}{N} \quad (5)$$

is the rms signal spectral variation over the rms spectral noise, or the spectral signal-to-noise. Since D/σ_D is this quantity times \sqrt{M} , it is evident that for sufficiently large M the detectable quantity can be estimated accurately even if local spectrum features are well below the noise level ($S/N \ll 1$).

D will be negative if the target gas is observed in absorption (is "cooler" than the background) and positive if it is observed in emission. Hence, detection of the target gas can be based on the test

$$|D'| \geq R_D \quad (6)$$

where R_D is some predetermined threshold. Knowing the statistics of D' (Eqs. 3 and 4) we can work out the statistics for $|D'|$ for both target present ($D \neq 0$) and target not present ($D = 0$), and finally determine a threshold R_D that yields satisfactory detection and false

detection probabilities. It can be shown that the threshold value

$$R_D = 2.58 \sigma_D = 2.58 \frac{\sqrt{2} \text{NESR}}{\sqrt{M} \sigma_b} \quad (7)$$

results in approximately 95 percent detection probability and approximately one percent false detection probability when D equals:

$$4.23 \sigma_D = 4.23 \frac{\sqrt{2} \text{NESR}}{\sqrt{M} \sigma_b} \equiv \text{MDQ} . \quad (8)$$

This, by definition, is the minimum detectable quantity.

The NESR, M and σ_b all vary with the spectrometer resolution $\Delta\nu$. A near-optimum value for $\Delta\nu$ is the halfwidth of the target gas spectral lines, which is $\sim 0.1 \text{ cm}^{-1}$ for targets near sea-level. That is, $\Delta\nu \approx 0.1 \text{ cm}^{-1}$ will give the smallest MDQ from Eq. (8). The single parameter in Eq. (8) that depends on the target gas and detection geometry is σ_b , the standard deviation of the reference spectrum τ_{bg} degraded to 0.1 cm^{-1} resolution.

FTS baseline system

The FTS baseline configuration that was selected uses a four-port Michelson interferometer with a single dichroic and two detector monoliths in each of the two output ports (see Fig. 1). This arrangement allows the simultaneous detection of up to four different target species. The fourth port (a second input port) provides for illumination of the backside of the interferometer beamsplitter by an internal blackbody reference or by a different (background) portion of the external scene than is viewed by the primary input port. Utilization of the fourth port in this manner effects an optical subtraction of the scene and reference blackbody spectra or of the displaced scene spectra, and, more important, results in a potentially large reduction in the interferogram dynamic range.⁴ If the reference blackbody and background have the same brightness temperature, the resultant target-background spectral contrast obtained by this optical scheme is the same as would be obtained using a conventional single-port interferometer and merely subtracting the outputs of two different mosaic elements. The details of the selected baseline configuration are given in Ref. 1.

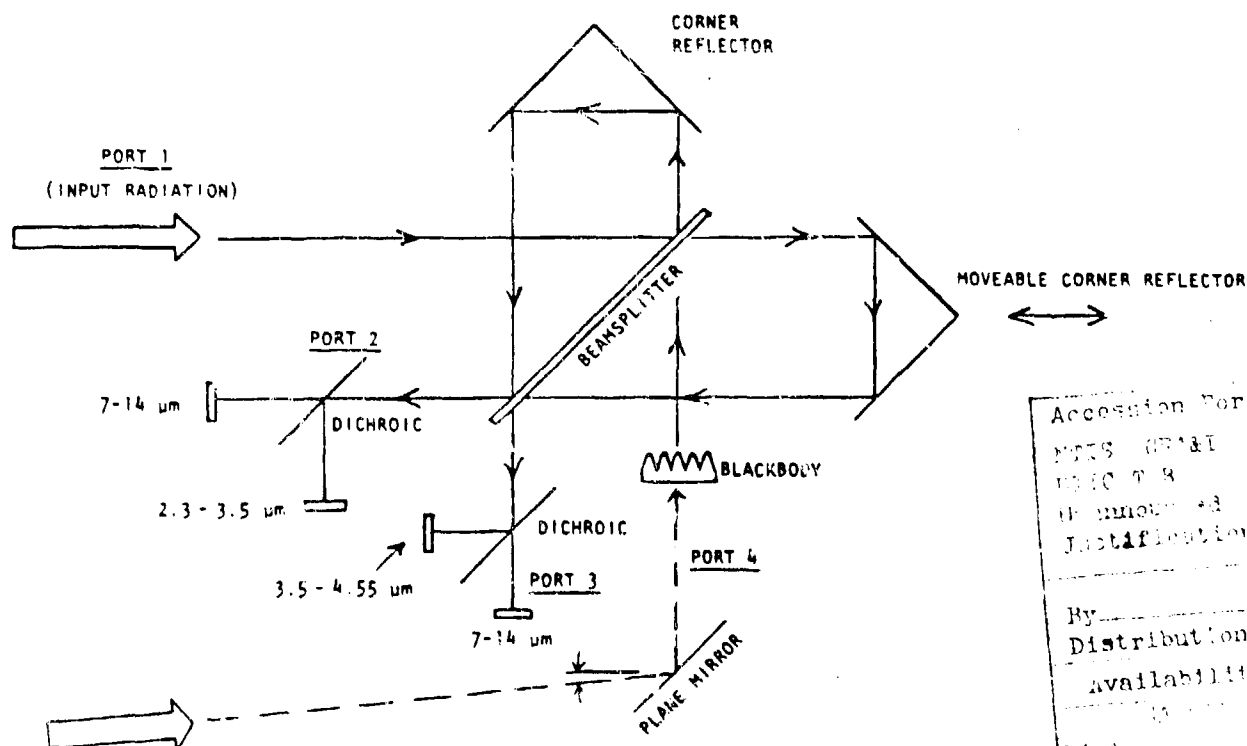


Figure 1. Optical layout for selected baseline configuration.

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MDQ and field test results

The MDQ's were calculated for several candidate detection bands of each of 14 different molecular species. The "best" band for each species was selected on the basis of the corresponding minimum detectable column thicknesses (MIN u's) for a given small temperature difference between target cloud and background. The relationship between MIN u and MDQ is, of course, strongly dependent on the spectral location of the detection band through the Planck function temperature derivative. Table 1 is a partial list of the best bands, the NESR's for a 10-second spectrum scan time, the corresponding MDQ and the MIN v. The last quantity is the minimum detectable concentration in ppmv for the conditions noted in the table footnote.

Table 1. MDQ and MIN v results

Gas	Band (cm ⁻¹)	*NESR (W/cm ² -sr-cm ⁻¹)	*MDQ (molec/cm ²) (W/cm ² -sr-cm ⁻¹)	**MIN v (ppmv)
HCl	2900-3000	1.3×10^{-9}	2.5×10^9	20
NO ₂	2850-2935	1.4×10^{-9}	1.3×10^{10}	92
DF	2700-2900	2.6×10^{-9}	3.5×10^9	17
HBr	2450-2650	3.9×10^{-9}	2.4×10^{10}	51
N ₂ O	2160-2210	3.1×10^{-9}	3.1×10^{10}	22
CO	2130-2185	3.6×10^{-9}	7.2×10^{10}	16
CH ₄	1295-1310	3.9×10^{-9}	2.1×10^{12}	163
SO ₂	1090-1210	1.5×10^{-8}	2.7×10^{11}	16
NH ₃	915-970	1.1×10^{-8}	2.0×10^{10}	1.0
HNO ₃	887.5-902.5	6.0×10^{-9}	3.4×10^{10}	1.6
C ₂ H ₄ O ₂	880-1000	2.0×10^{-9}	5.7×10^{10}	2.8
CH ₃ I	790-990	2.4×10^{-8}	6.7×10^{11}	32
NO ₂	710-795	1.3×10^{-8}	4.0×10^{11}	19

Note that the MDQ scales as the system NESR (Eq. 8). The more fundamental quantity σ_b for each detection band can be determined from Eq. (8) and the third and fourth columns of Table 1. The number M is equal to the width of the band divided by 0.1 cm⁻¹. The σ_b 's and MDQ's correspond to a vertical path through most of the Midlatitude Summer model atmosphere.

Field measurements were performed at Utah State University to validate the theoretical predictions. In the experiment a model stack emitting a controlled flow of N₂O in front of a heated "background" plate was observed by an FTS system at a distance of 273 meters. The detection band selected for the experiment is 2170-2260 cm⁻¹, which includes most of the ν_3 band of N₂O (this is a better N₂O detection band than the one given in Table 1 for the measurement geometry of the experiment). The N₂O was successfully identified and quantified in repeated trials when the detectable quantity was slightly greater than the calculated MDQ. Figure 2 shows a computed (FASCOD1) reference contrast spectrum for one of the data runs, and two examples of measured contrast spectra that resulted in N₂O detection. The middle panel of the figure shows the measured contrast when the detectable amount is approximately four times the MDQ; in the bottom panel the detectable amount is ~1.5 times the MDQ. There is extremely high probability of detection (>> 0.95) when the detectable amount is 1.5 times the MDQ, even though the measured contrast spectrum for this amount looks like noise. The spectrum signal-to-noise defined by Eq. (5) is 0.26 for the bottom panel in Fig. 2; at the MDQ level the S/N would be 0.15.

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*For baseline system and dwell time = 10 secs.

**MIN v = minimum detectable volume concentration for $t_d = 10$ secs., cloud thickness = 10 m, $\Delta T = 5^\circ\text{C}$., $T_{\text{sf}} = 300\text{K}$.

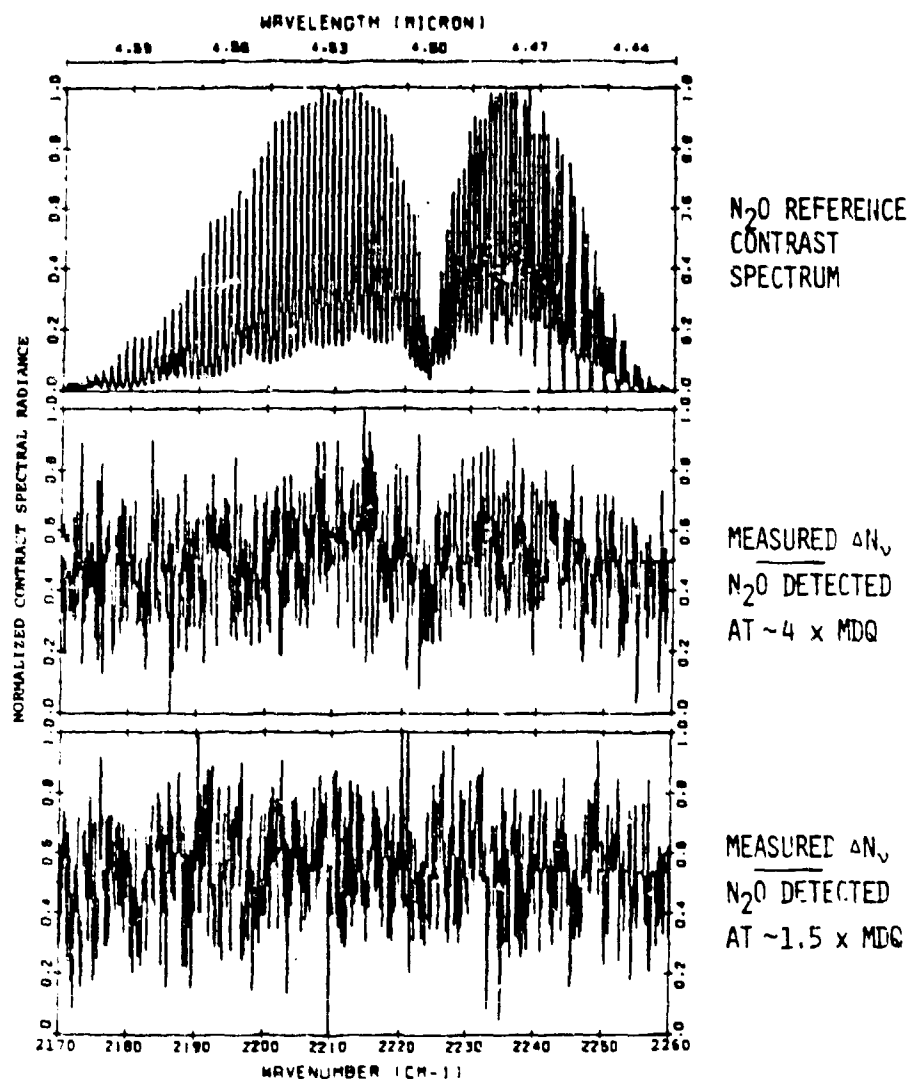


Figure 2. Normalized reference contrast spectrum for ν_3 band of N₂O (top panel) and two normalized contrast spectra obtained from measurements.

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